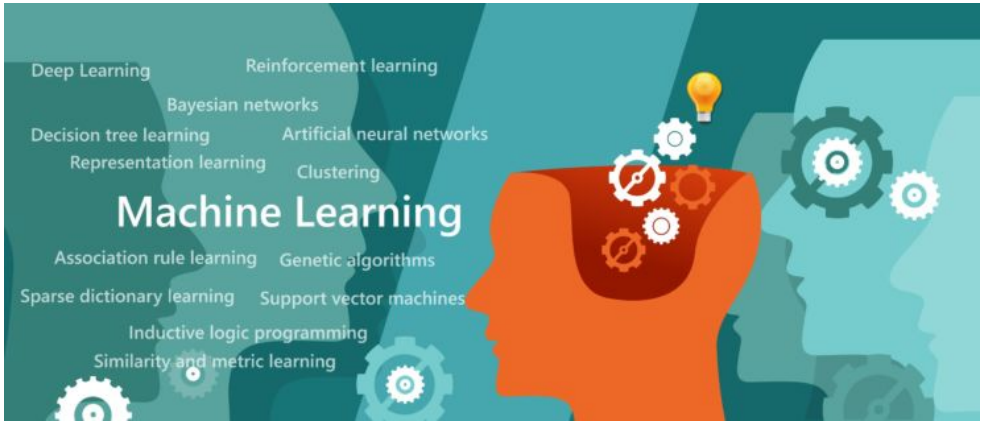
# CSCE 421 - Machine Learning

## Lecture 1 - Welcome!

# Welcome to CSCE 633!

- About this class
- Introduction to Machine Learning
  - What is Machine Learning?
  - Basic concepts



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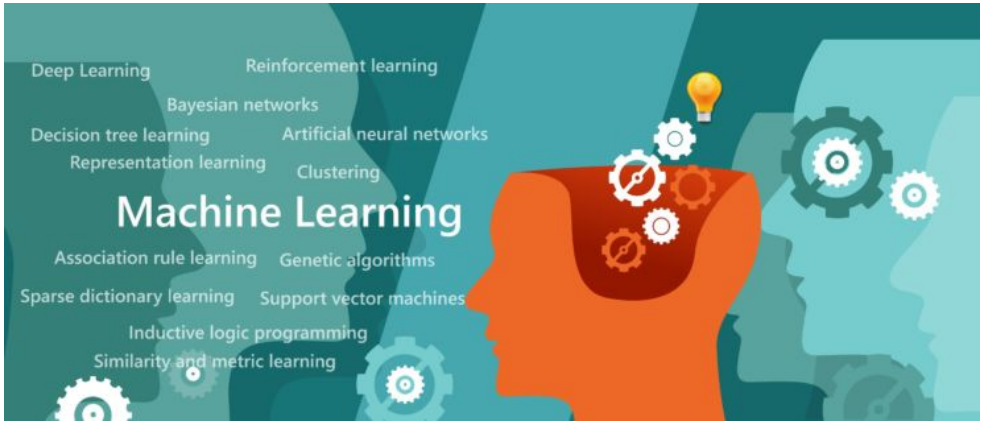


# Welcome to CSCE 633!

- Instructor
  - Theodora Chaspari
  - chaspari@tamu.edu (but use Piazza for quickest reply)
  - Office: 322D HRBB
  - Office Hours: Monday, 3.00pm-5.00pm

- TA
  - Zhenyu Wu
  - wuzhenyu_sjtu@tamu.edu
  - Office: 407 HRBB
  - Office Hours: Tuesday & Thursday, 9.00-10.00am

# Class websites

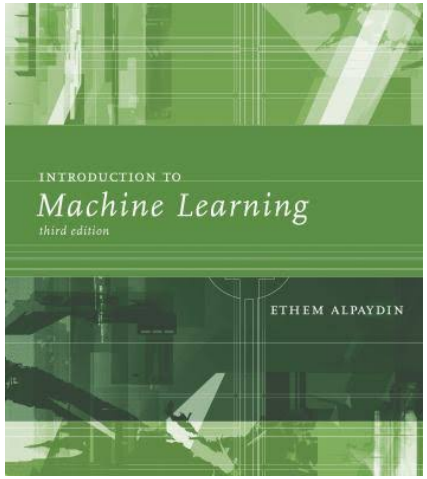
- Piazza
  - piazza.com/tamu/fall2019/csce421/home
  - Class logistics
  - Class discussions
  - Lecture slides
  - Homework posting, homework solutions
  - Quiz/exams material
  - For sending private messages to me, the TA, or the grader

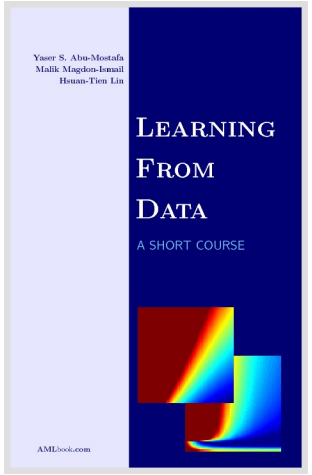
- E-campus
  - For uploading homeworks and posting grades

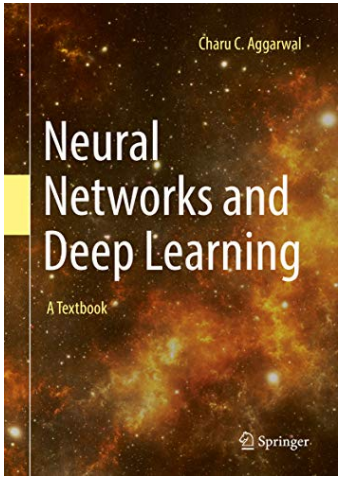
- Google drive (for supplementary material)
  - https://drive.google.com/open?id=1BXwughTmKtN-Ch3bBykpCMwee6BEXQ9s
  - Lecture videos (when needed)
  - Updated roadmap

# Textbook and course material

- Lecture notes
- Textbook
  - Introduction to Machine Learning, Ethem Alpaydin
  - Learning from Data, Yaser S. Abu-Mostafa
  - Neural Networks and Deep Learning, Charu Aggarwal
- Supplemental materials



# Class structure

- 5 homework sets (50%)
  - 1% penalty on late submission per assignment
- 2 exams (2x15%=30%)
  - Midterm: October 14th (during class time)
  - Final: December 6th (7.30-9.30am)
- 5 quizzes, 4 best added (4x5%=20%)
  - Almost biweekly
  - Exact dates to be determined based on class pace
  - This will help us all be at the same page!

# Homework Submission

- All homeworks will be submitted as a **single pdf** on eCampus
  - The executable code (if required) needs to be included in the pdf
- Programming assignments
  - You can use C/C++, Python, Matlab (or Octave)
- Math assignments
  - Please submit solution produced in Latex
  - Or **very clear** handwritten solution
  - This will help our TA a lot.

# Active Learning

- Would you ever take a cardio class without actually participating in it?
- So why take a CS course without practicing the material in class?

# Active Learning

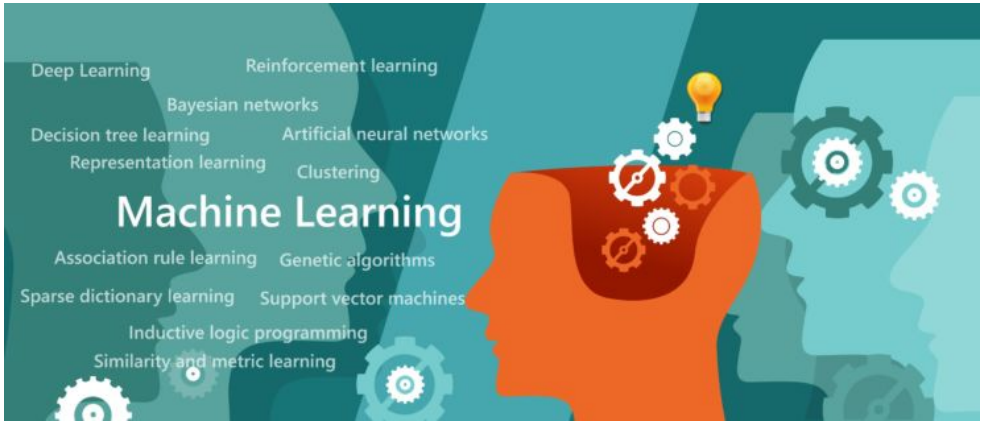
- "Anything that involves students in doing things and thinking about the things they are doing" (Bonwell & Eison, 1991)
- "Anything course-related that all students in a class session are called upon to do other than simply watching, listening and taking notes" (Felder & Brent, 2009)
- Audience attention starts to wane after 10-20 mins
- Research suggests that incorporating active learning techniques
  - encourages student engagement
  - reinforces important material, concepts, etc.
  - builds self-esteem
  - creates a sense of community

# Active Learning

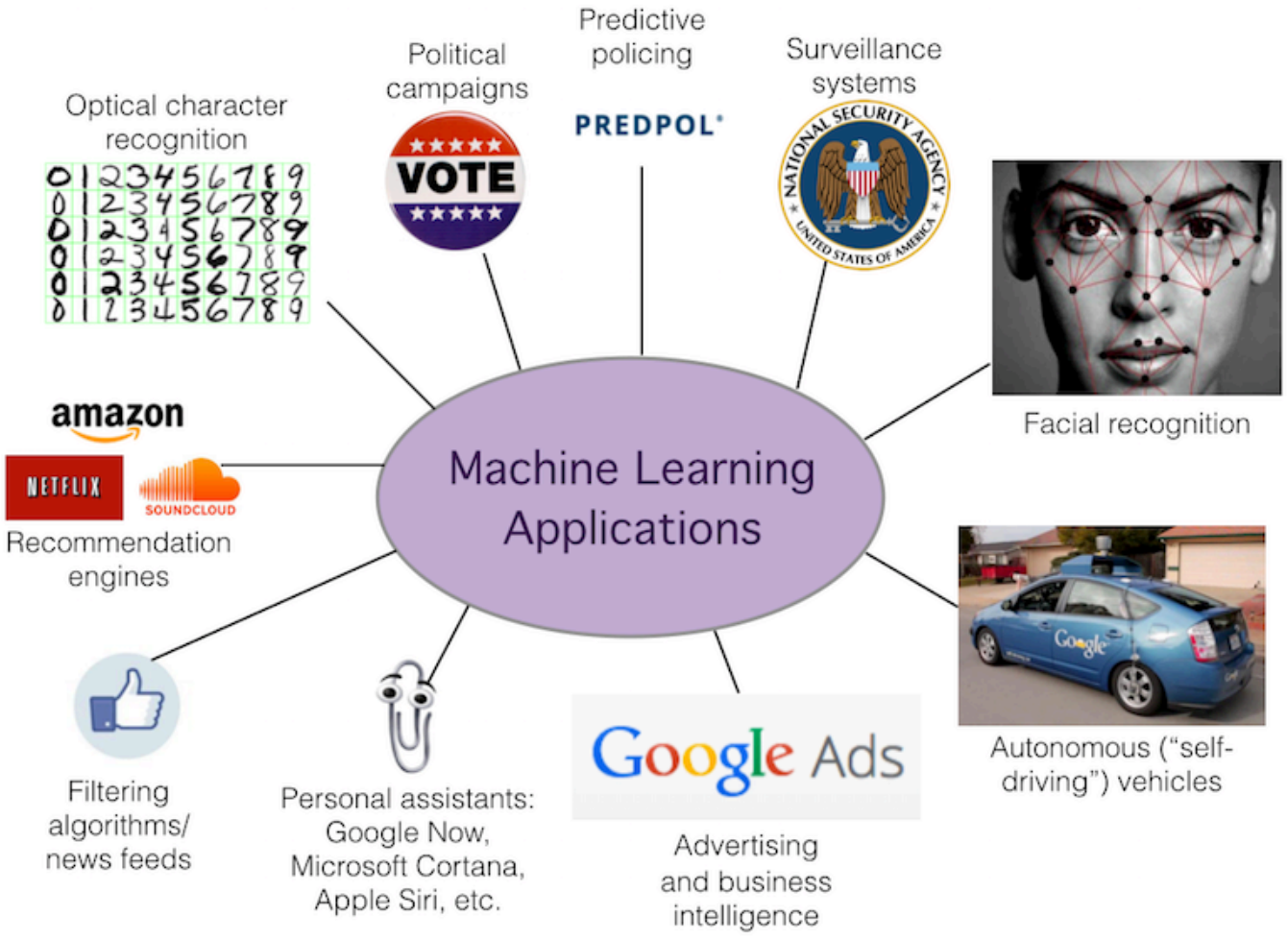
- Kahoot: free software platform that will help us answering multiple choice questions during class
- https://kahoot.it/#/
- Google Play, Apple Store
- You won't be graded in any of these
- Just a fun way to engage and participate more in class 🙂

# Outline

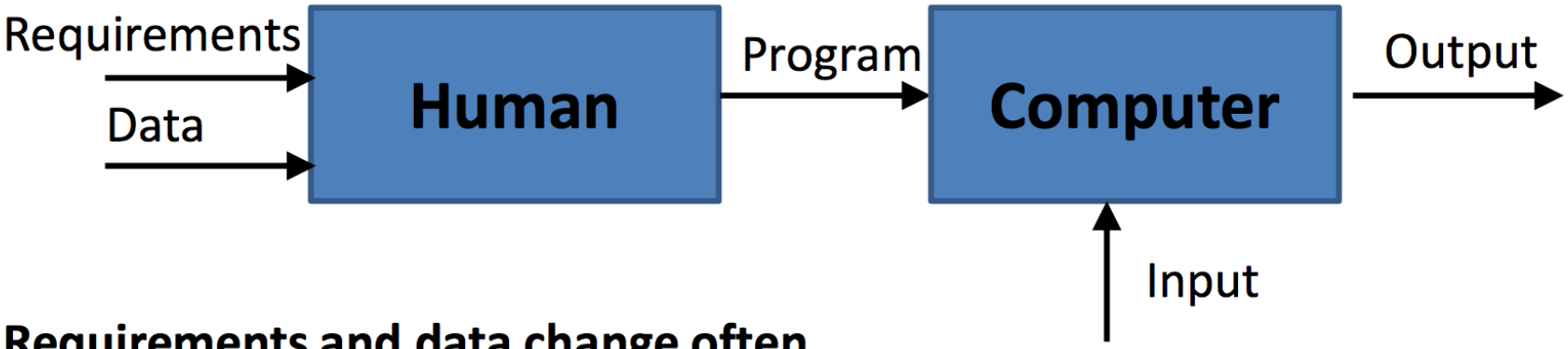
- About this class
- Introduction to Machine Learning
  - What is Machine Learning?
  - Basic challenges



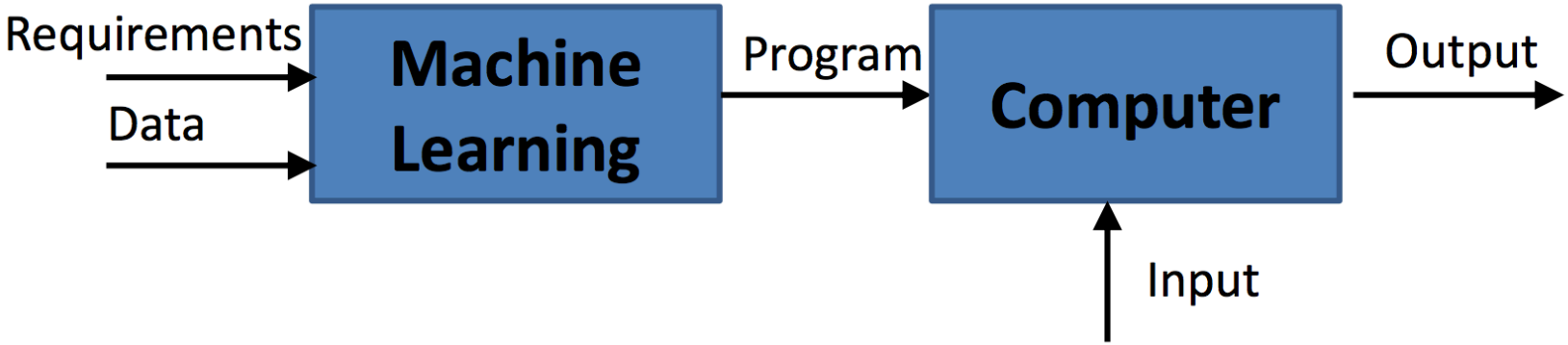
# Machine learning is everywhere



# What is machine learning?




**Requirements and data change often**




**Big Data:** 40 billion webpages, 100 hrs YouTube video uploaded every 1min, 1 million Walmart transactions per hour

# What is machine learning?

*A possible definition*[1]

A set of methods that can automatically detect patterns in data, and then use those to predict future data or perform other kinds of decision making under uncertainty.

*A more formal definition*[2]

A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T as measured by P improves with experience E

[1] From K.P. Murphy
[2] From T. Mitchell

# What is machine learning?

**Definition:** A computer program learns from experience E with respect to some task T and some performance measure P, if its performance on T as measured by P improves with experience E

**Question:** Suppose your Facebook account watches the users added to your friends' list. Based on that, it learns how to suggest new friends for you. What is task T in this setting?

A. Classifying a user X according to whether or not you would possibly send them a friend request
B. Identifying the characteristics of users to which you send a friend request
C. Computing the percentage of suggested users to whom you actually sent a friend request
D. All of the above

# What is machine learning?

**Definition:** A computer program learns from experience E with respect to some task T and some performance measure P, if its performance on T as measured by P improves with experience E

**Question:** Suppose your Facebook account watches the users added to your friends' list. Based on that, it learns how to suggest new friends for you. What is task T in this setting?

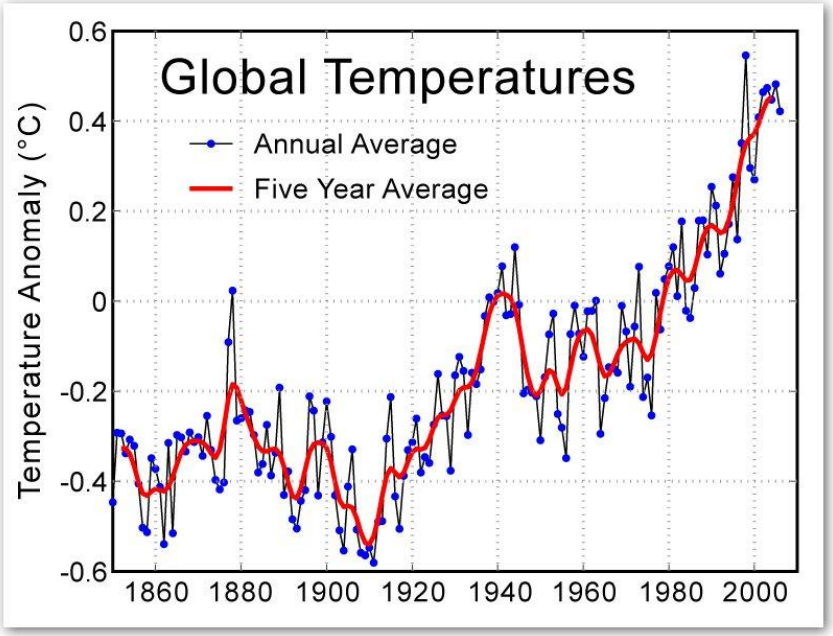
A. Classifying a user X according to whether or not you would possibly send them a friend request (task T)
B. Identifying the characteristics of users to which you send a friend request (experience E)
C. Computing the percentage of suggested users to whom you actually sent a friend request (performance measure P)
D. All of the above

# Key ingredients for a machine learning task

- Data
  - collected from past observations (training data)
- Model
  - devised to capture patterns in data
  - doesn't have to be absolutely true, as long as it is close enough
  - should tolerate randomness & mistakes, i.e. uncertainty
- Prediction
  - apply the model to
    - forecast what is going to happen in the future
    - automatically make a decision for unknown data, etc.

# Example: Detecting Patterns

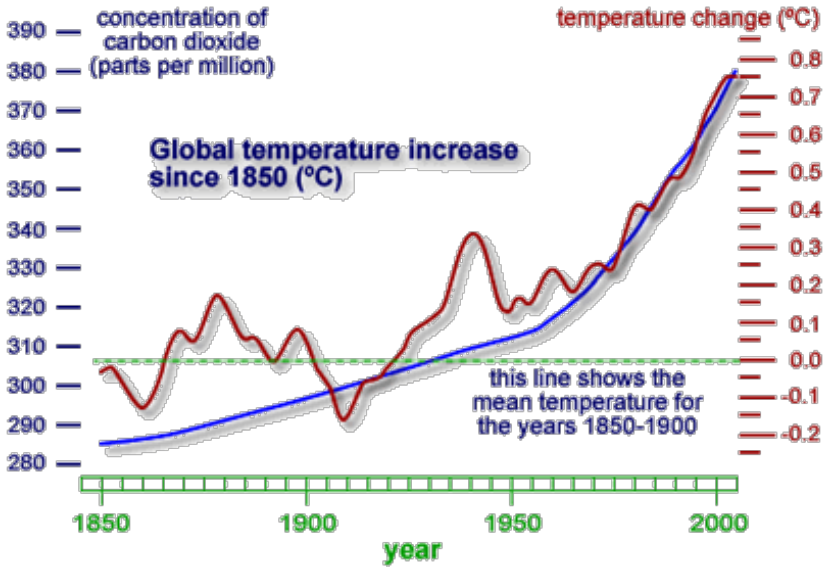
How has the temperature been changing over the last 140 years?




- Generally increasing patterns
- Local oscillations

# Example: Describing Patterns

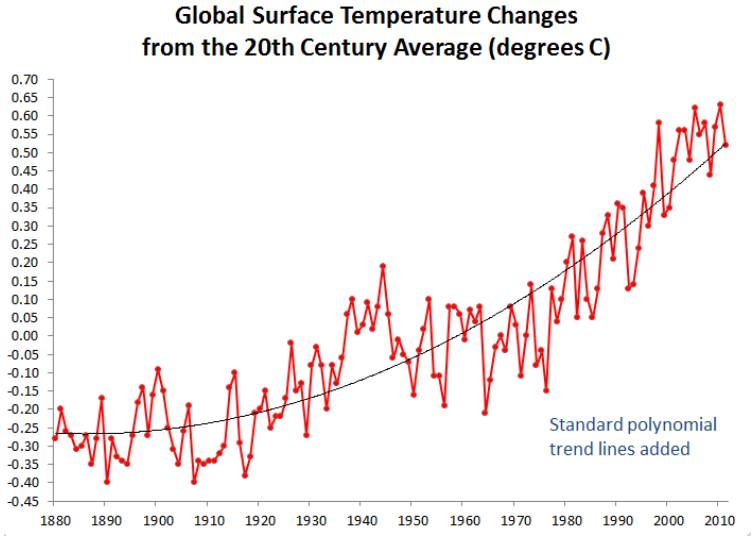
Build a model: fit the data with polynomial function




- Quadratic model is not accurate for every year
- But captures the general trend

# Example: Predicting Future Value

## What is the temperature of 2010?




- Again the model is not accurate for that specific year
- But it is close enough

# The three components of learning

| Representation | Evaluation | Optimization |
|---|---|---|
| Instances | Accuracy/Error rate | Combinatorial optimization |
| *K*-nearest neighbor | Precision and recall | Greedy search |
| Support vector machines | Squared error | Beam search |
| Hyperplanes | Likelihood | Branch-and-bound |
| Naive Bayes | Posterior probability | Continuous optimization |
| Logistic regression | Information gain | Unconstrained |
| Decision trees | K-L divergence | Gradient descent |
| Sets of rules | Cost/Utility | Conjugate gradient |
| Propositional rules | Margin | Quasi-Newton methods |
| Logic programs | | Constrained |
| Neural networks | | Linear programming |
| Graphical models | | Quadratic programming |
| Bayesian networks | | |
| Conditional random fields | | |

a learner must be represented in some formal language

an evaluation function assesses the performance of a learner

find the highest-scoring learner

Source: P. Domingos, 2014

# Types of Learning

- Supervised (or predictive) learning
  - learn mapping of inputs to outputs given a set of labelled pairs
  - training data includes desired outputs
  - obvious error metrics, e.g. prediction accuracy
  - cancer prediction, stock prices, house prices, spam detection
- Unsupervised (or descriptive) learning
  - find hidden/interesting structure in data ("knowledge discovery")
  - training data does not include desired outputs
  - less well-defined problem with no obvious error metrics
  - topic modeling, market segmentation, clustering of hand-written digits, news clustering (e.g. Google news)
- Reinforcement learning
  - the learner interacts with the world via actions
  - finds the optimal policy of behavior based on "rewards" it receives
  - robot navigation, game playing, self-driving cars

# Supervised Learning

- Learning a mapping from inputs $\mathbf{x_i}$ to outputs $y_i$ given a labelled set of input-output pairs (N samples)

$$\mathcal{D} = \{(\mathbf{x_i}, y_i)\}_{i=1}^{N}$$

- Data Matrix (N samples, D features)

$$\mathbf{X} = [\mathbf{x_1^T} \ldots \mathbf{x_N^T}] \in \Re^{D \times N} \qquad \mathbf{x_i} \in \Re^{1 \times D}$$

- Function approximation, function f is unknown and we approximate it

$$y = f(\mathbf{x})$$

- Classification
  - $y_i$ is categorical or nominal (C classes): $y_i \in \{1, \ldots, C\}$
- Regression
  - $y_i$ is a real-valued scalar: $y_i \in \mathbb{R}$

# Supervised Learning: Classification

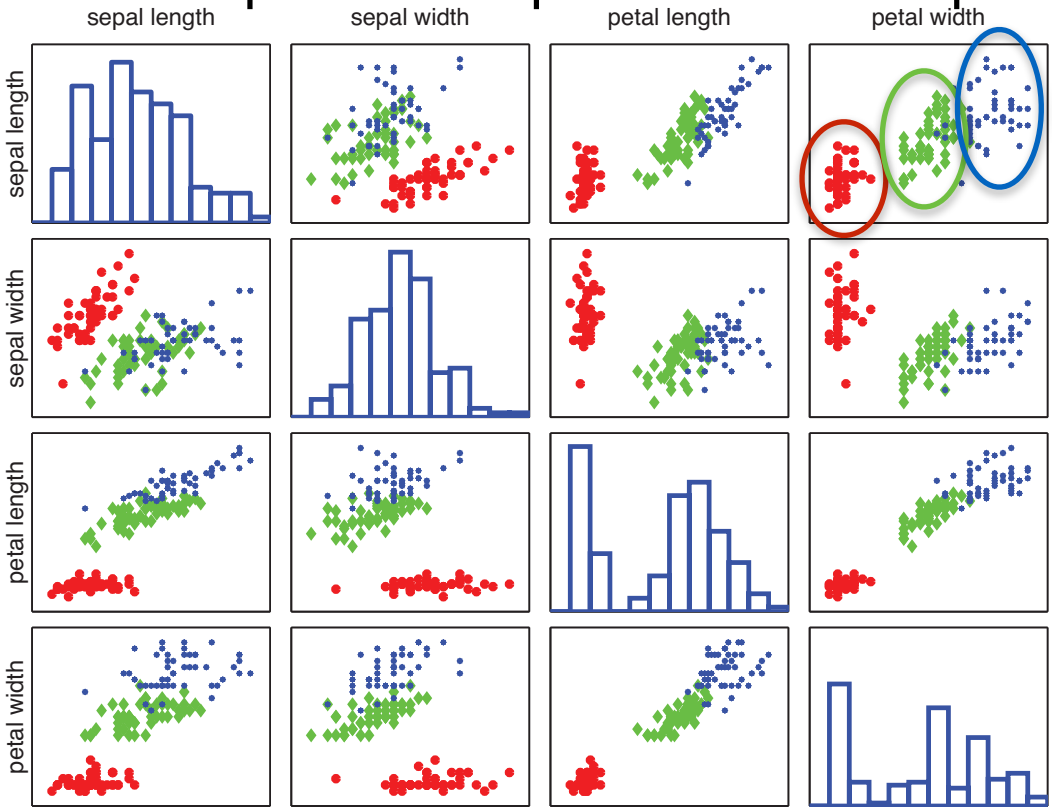
## Recognizing types of Iris flowers (by R. Fisher)

setosa "●"

versicolor "◆"

virginica "✳"

Scatter plots of all possible feature pairs




Exploratory data analysis (intuition)

# Supervised Learning: Classification

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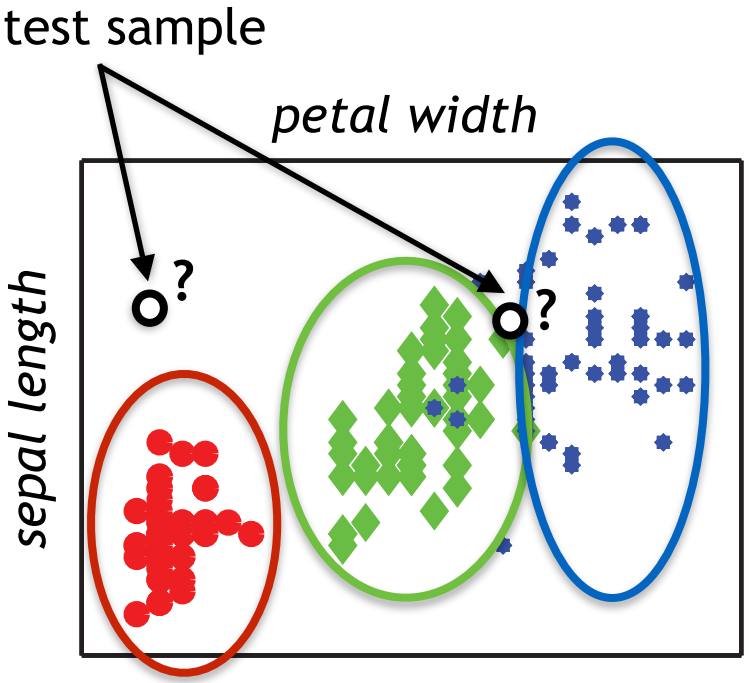


### K-Nearest Neighbor (K-NN) classifier

- Test sample **x** is assigned to the most common class among its neighbors [N]

$$y = f(\mathbf{x}) = arg \max_{c=1,\ldots,C} v_c$$

most common class

number of votes from class c

# Brief probability review

**Probability**

- P(A): probability that event A is true
  - A: “it will rain tomorrow”
  - p(A)=0.2: “there is 20% chance of rain tomorrow”

**Conditional probability**

- P(A|B): probability of event A, given that event B is true
  - A: “it will rain tomorrow”
  - B: “today is humid”, C: “today is windy”
  - p(A|B): “chance of rain tomorrow, given that today is humid”, e.g. p(A|B)=0.6
  - p(A|B∧C): “chance of rain tomorrow, given that today is humid and windy”, e.g. p(A|B∧C)=0.7

# Supervised Learning: Classification

## Recognizing types of Iris flowers (by R. Fisher)

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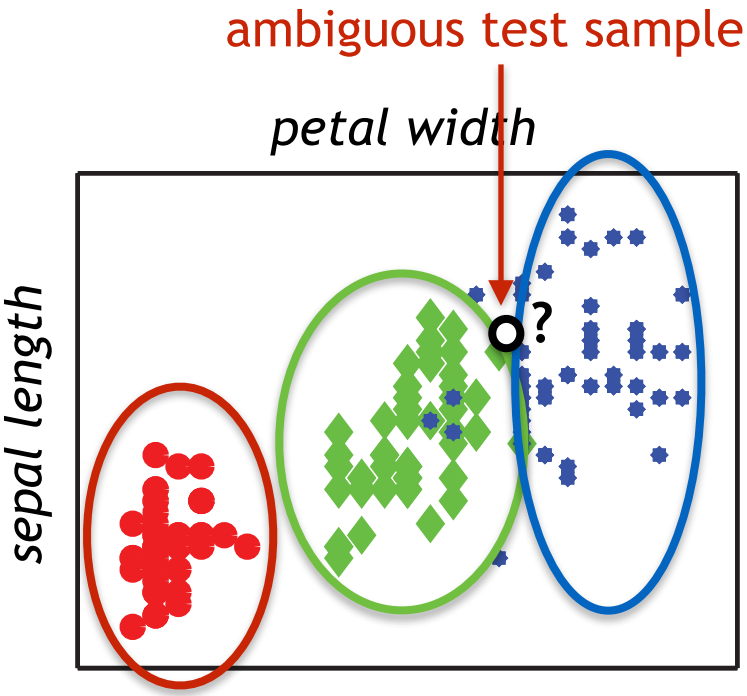



## The need of probabilistic predictions

- The right class of testing samples is unclear
- Return probabilities to handle ambiguity

$$y = f(\mathbf{x}) = arg \max_{c=1,\ldots,C} p(y = c|\mathbf{x}, \mathcal{D})$$

most **likely** class

**posterior probability:** probability of test sample belonging to class c given input vector **x and** training set D

**MAP estimate (maximum a posteriori)**

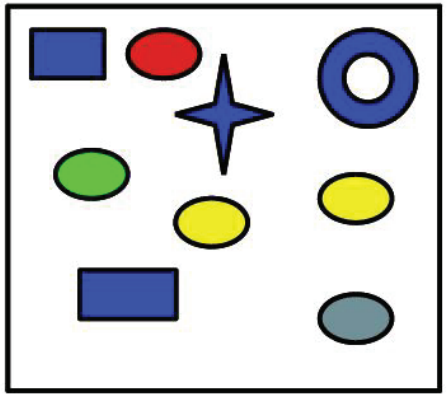
Biomedical applications (e.g. tumor classification)
DeepQA for IBM Watson, etc.

# Why is it important to model uncertainty?

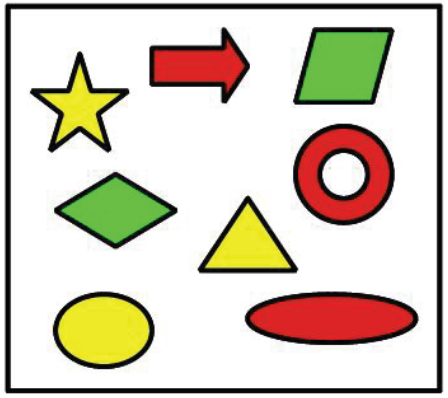
**Question:** Given the training data bellow, what would be a reasonable probability that a classifier would assign to the following test samples?

**Training Set D**

**Class A**



**Class B**



**Test Set**

Test sample s1: 

Test sample s2: 

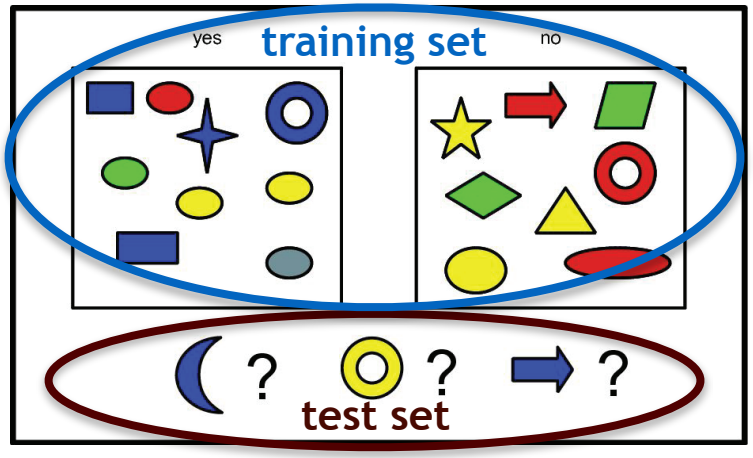
**A.** $P(s1 \in A \mid D)=0.9,\ P(s2 \in A \mid D)=1$

**B.** $P(s1 \in B \mid D)=0.9,\ P(s2 \in B \mid D)=0.1$

**C.** $P(s1 \in B \mid D)=0.9,\ P(s2 \in A \mid D)=0.5$

**D.** None of the above

# Why is it important to model uncertainty?




D features (attributes)

N cases

| Color | Shape | Size (cm) | Label |
|---|---|---|---|
| Blue | Square | 10 | 1 |
| Red | Ellipse | 2.4 | 1 |
| Red | Ellipse | 20.7 | 0 |

discrete features

continuous features

training labels

- Required to generalize beyond the training set
- The right class of the testing samples is unclear
- To handle such ambiguous cases we can return a probability instead of a hard 0/1 decision

# Unsupervised Learning

- Discovering structure (patterns, regularities, etc.) in “unlabelled” data
- Density estimation: we want to see what generally happens and what not

$$p(\mathbf{x_i}|\boldsymbol{\theta})$$

instead of $p(y_i|\mathbf{x_i};\boldsymbol{\theta})$ (supervised learning)

- Clustering
  - identifying sub-populations in the data
- Dimensionality reduction
  - project data to a lower dimensional subspace capturing its essence
- Matrix completion
  - data imputation to infer values of non-existing entries

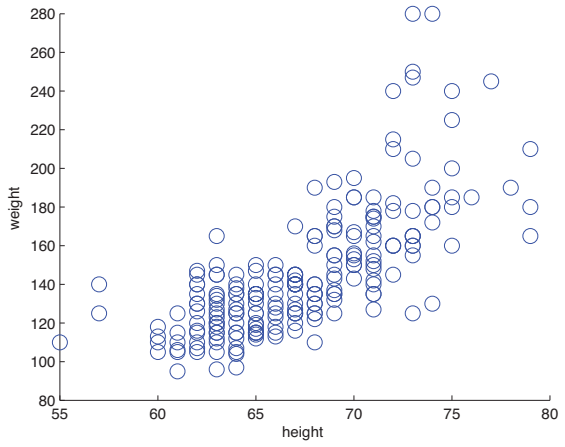
# Unsupervised Learning: Clustering

- Step 1: Estimate the distribution over the number of clusters

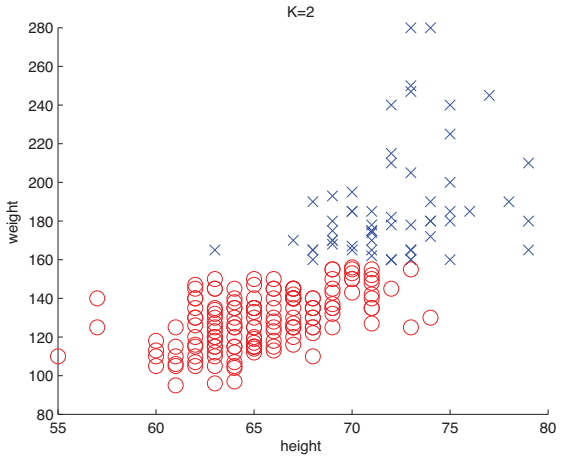
$$p(K|\mathcal{D})$$

- Step 2: Estimate which cluster each point belongs to

$$z_i^* = arg \max_{k=1,\ldots,K} p(z_i = k|\mathbf{x_i}, \mathcal{D})$$



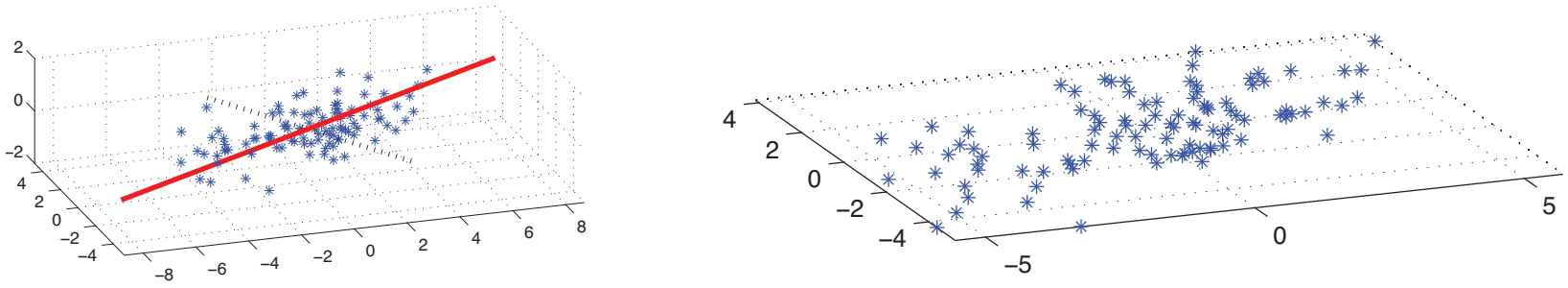

(a)




(b)

# Unsupervised Learning: Dimensionality Reduction

- Lower dimensional representations can have better predictive power
  - minimized data redundancies
  - avoiding “curse of dimensionality”




(a) (b)

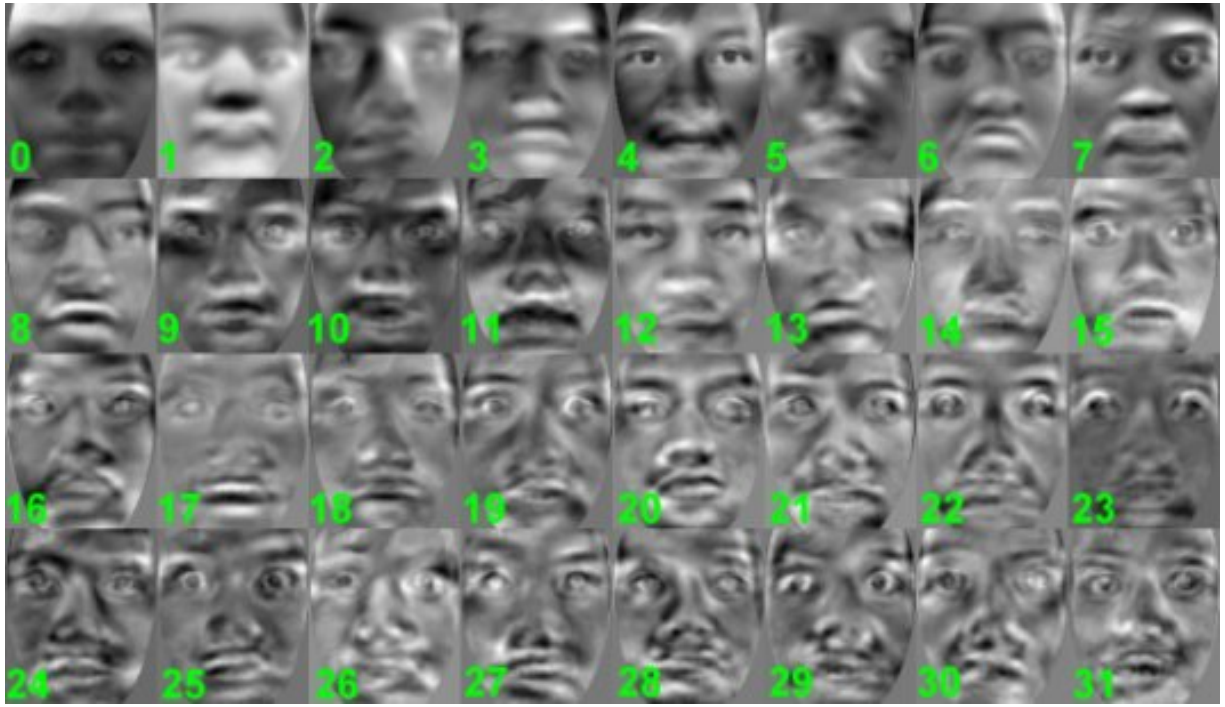
**Principal component analysis (PCA)**

identifies a set of uncorrelated axes that maximize the variance of the data

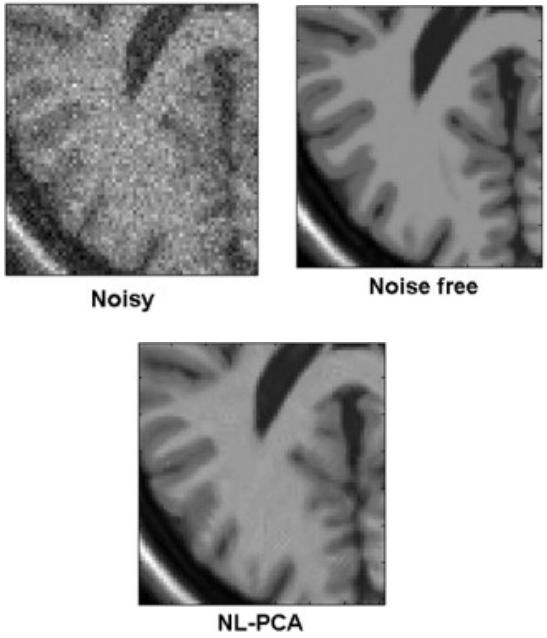
# Unsupervised Learning: Dimensionality Reduction

## Example applications of PCA

### Eigenfaces

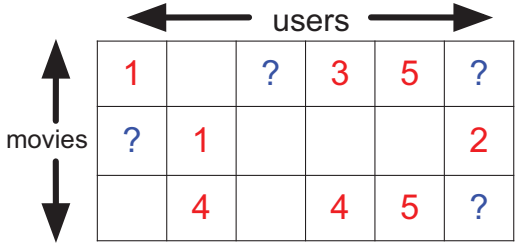



### MRI denoising



# Unsupervised Learning: Matrix completion

## Recommender systems




Customers Who Bought This Item Also Bought


## Image restoration


Sources: Wang & Jia, 2017;
Papandreou, Maragos, & Kokaram, 2008

# To sum up

- Machine learning definition
- Key components of learning: representation, evaluation, optimization
- Types of learning systems: supervised & unsupervised
- Challenges in machine learning

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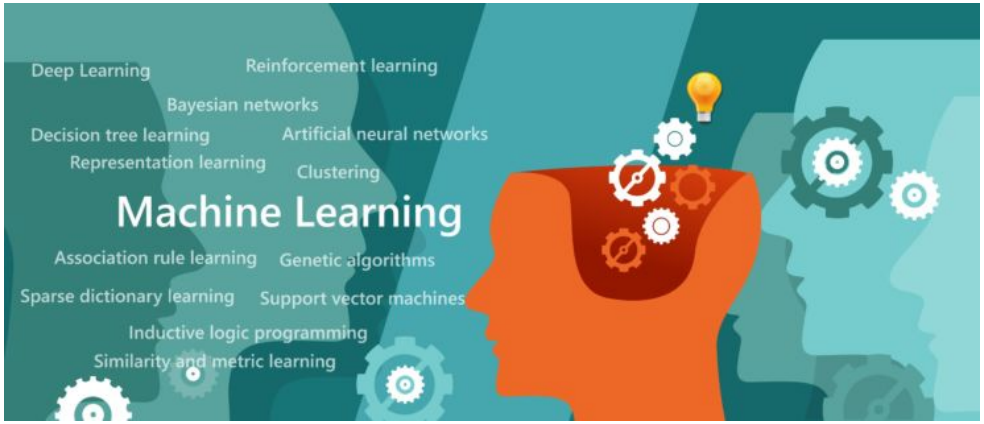
  - Basic challenges

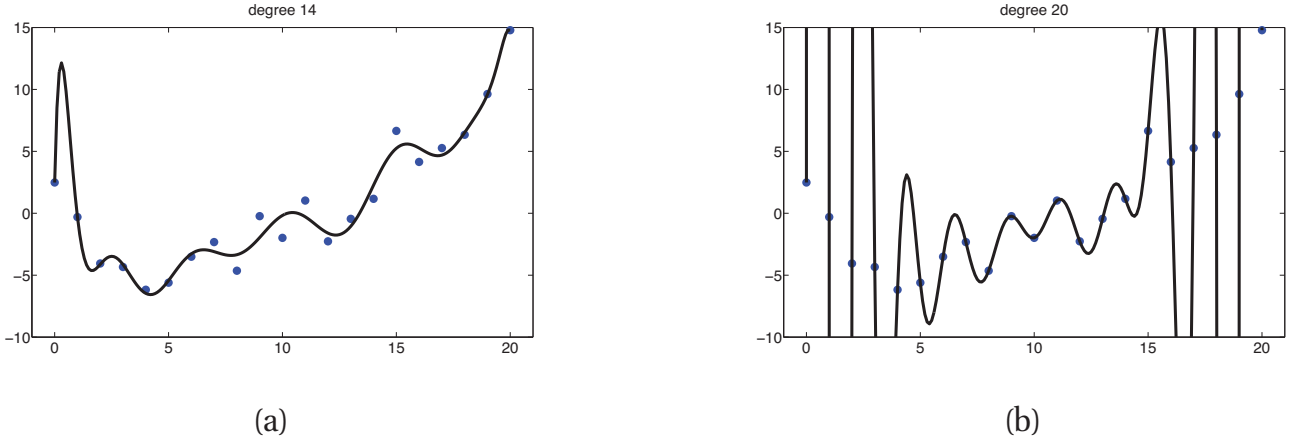


# Key Machine Learning Challenges
## Generalization

- Biggest ML challenge is to generalize beyond the training set
- **Never evaluate your ML system on the train data only**
  - Use test data instead
- Contamination of the ML system from the test data can occur when:
  - use test through excessive parameter tuning
    - Avoid this with (**cross-)validation**
- On the positive side 🙂
  - We may not need to fully optimize it, since the objective function is only a proxy of the true one

# Key Machine Learning Challenges
## Overfitting

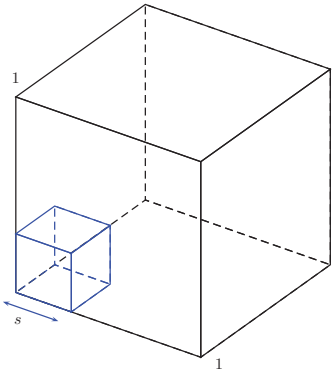
- The risk of using highly flexible (complicated) models without having enough data
- Ways to avoid overfitting
  - (cross-)validation
  - regularization



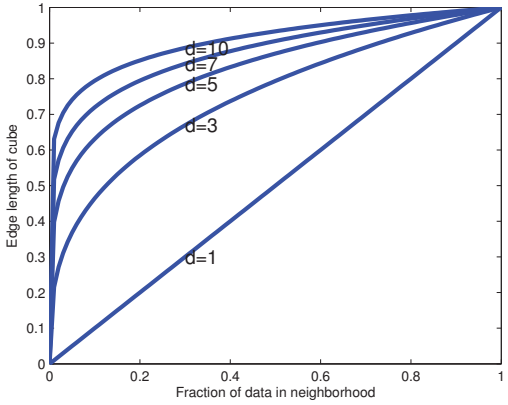

*Example of polynomial fit*

# Key Machine Learning Challenges
## Curse of dimensionality

- All intuition fails in higher dimensions
- For a fixed training set, generalization gets harder in larger dimensions
  - harder to systematically search a high-dimensional grid-space
  - harder to accurately approximate a high-dimensional function
- On the positive side 🙂
  - "blessing of non-uniformity": examples aren't usually spread uniformly



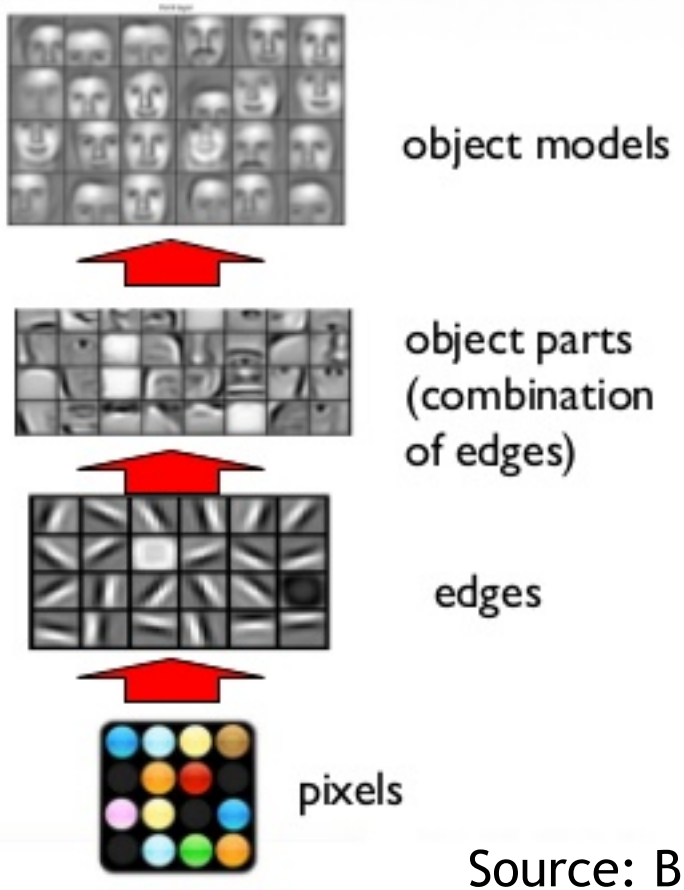

(a)




(b)

# Key Machine Learning Challenges
## Feature Engineering

- Learning is easy if you have informative features for the problem
- Automating the feature engineering process
  - Deep learning systems producing output from raw input




Source: Baidu

# Key Machine Learning Challenges
## "No-free-lunch" theorem

- "All models are wrong but some models are useful", G. Box, 1987
- There is no single best ML system that works optimally for all kinds of problems
- On the positive side 🙂
  - General assumptions can actually work pretty well, e.g.
    - Similar examples belong to similar classes
    - Independence and smoothness assumptions
- We might need to try lots of different ML systems and learning algorithms to cover the wide variety of real-world data.
- Machine learning is not magic: it can't get something out of nothing, but it can get more from less!

# To sum up

- Machine learning definition
- Key components of learning: representation, evaluation, optimization
- Types of learning systems: supervised & unsupervised
- Challenges in machine learning

Readings:

- Alpaydin Ch1, Abu-Mostafa Ch 1
- P. Domingos, "A few things to know about machine learning"
- **For next class:** Please take a look at the Linear Algebra Review Handout (uploaded on Piazza)

Fun videos to watch:

- https://www.youtube.com/watch?v=R9OHn5ZF4Uo
- www.youtube.com/watch?v=ujxriwApPP4